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Crystal field at the impurity center sites in ionic crystals

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Abstract

Perturbation theory is developed for second-quantized operators in a basis of partly nonorthogonal orbitals. This method may be helpful in carrying out ab initio calculations of the parameters of the crystal field at the impurity center sites. As an illustration, when estimating the crystal field parameters for Yb3+: KZnF3, some fitting parameters are calculated using this method. The results agree well with experimental data, which indicates that this theory shows considerable promise. © 2005 Pleiades Publishing, Inc.

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